

Coexistence of CDW with staggered superconductivity in a ferromagnetic material

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Abstract. - In usual superconductivity (SC), the pairs have zero total momentum irrespective of their symmetry. Staggered SC would involve, instead, pairs with a finite commensurate total momentum, but such exotic states have never been proven to be realized in nature. Here we study for the first time the influence of particle-hole asymmetry on the competition of staggered SC with Charge Density Waves (CDW) in a ferromagnetic medium. We obtain unprecedented situations in which CDW and staggered SC *coexist*. We also obtain cases of a SC dome near the collapse of a CDW state as well as cascades of transitions that exhibit remarkable similarities with the pressure phase diagram in UGe₂ suggesting that SC in this material may be *staggered* coexisting and competing with a CDW state.

The field of unconventional superconductivity (SC) is an extraordinarily rich source of challenging problems for fundamental and applied physics. High- T_c cuprates, heavy fermion materials, borocarbides and organic SC are examples of unconventional SC. A multitude of unconventional SC states have been proposed but only few have been proven to be realized in real material systems. Singlet or triplet unconventional SC states considered as realized so far are characterized by a zero total momentum of the pairs indicating in fact that the superfluid density is homogeneous in momentum space. In the present Letter we suggest that the surprising ferromagnetic (FM) SC state of UGe₂ is instead *staggered*, in which case the pairs have a *finite total momentum*. We also prove that staggered SC may *coexist* with charge density wave (CDW) states explaining features of the pressure phase diagram in UGe₂ and opening a new perspective for the discussion of other unconventional SC.

The unexpected discovery of SC well inside the *itinerant* FM state of UGe₂ under pressure [1] and subsequently in ZrZn₂ [2] and URhGe [3] represent a fascinating challenge for our understanding of SC [4–12]. The kind of unconventional SC involved as well as the complexity of the pressure phase diagrams in UGe₂ remain a puzzle. In fact, below $T_C(0) = 52$ K an almost fully polarized FM state is observed. Applying hydrostatic pressure, FM is suddenly eliminated at $p_{c2} = 1.5$ GPa. Around $p_{c1} = 1.1$

GPa, SC appears and at the optimum $p^* = 1.2$ GPa one finds $T_c(p^*) \leq 1$ K. This is well in the FM state where the Curie temperature and FM moment are still significant with $T_C(p^*) \simeq 30$ K, i.e. 60% of the original $T_C(0)$. In addition to SC, presumably another phase is present inside the FM state below $T^*(0) = 30$ K, and $T^*(p)$ also decreases with pressure until at p^* it hits the optimum $T_c(p)$ of the SC dome [8, 13]. The nature of the T^* phase is not clear, one possibility that we adopt here is to associate it with a charge density wave (CDW) [1, 8, 14, 15], a scenario supported also by LDA+U calculations [16]. This would explain the associated experimentally observed heat-capacity anomalies [17] and jumps in the magnetization on crossing the T^* phase boundary [13]. Finally, recent NQR experiments suggest that the T^* phase survives even below the SC transition dividing the SC dome into two parts: a low pressure part where SC and the T^* order coexist and a high pressure part where there is no signature of the T^* order [18, 19].

We explore in this Letter the *competition of staggered SC (i.e. zone boundary SC) with CDW* in a strong ferromagnetic background, a situation that has never been considered before. In fact, all previous theoretical investigations of SC in UGe₂ considered zero momentum (or zone center) SC. Note that the possibility of the relevance of staggered SC states for some heavy fermion compounds has first been considered in the past by D.L. Cox and

coworkers [20] in the context of a Ginzburg-Landau approach. Moreover, the SC pairing of spinless (or single-spin) fermions has been introduced in [21] and discussed within a Ginzburg-Landau theory. Here we start from a mean field BCS-type Hamiltonian

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} - \sum_{\mathbf{k}} (W_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}+\mathbf{Q}} + h.c.) - \sum_{\mathbf{k}} (\Delta_{\mathbf{k}}^0 c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}}^{\dagger} + h.c.) - \sum_{\mathbf{k}} (\Delta_{\mathbf{k}}^{\mathbf{Q}} c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}-\mathbf{Q}}^{\dagger} + h.c.) \quad (1)$$

The first term describes a 2D tight binding FS whose nesting properties with a wave vector $\hat{\mathbf{Q}}=(\pi, \pi)$ are controlled by the ratio of n.n. (t_1) and n.n.n. (t_2) hopping matrix elements. For $t_2/t_1 < 1$ the nesting with $\hat{\mathbf{Q}}$ is removed completely and the FS changes its shape. This is a schematic model for the destruction of nesting of the LDA+U Fermi surface [16] under pressure. There are several possibilities of competing SC and CDW orders described by the gap functions W and Δ in Eq.(1). They are related to the effective interactions via gap equations like Eqs. (2,3). The effective interactions $V_{\mathbf{k},\mathbf{k}'}^{SC}$ and $V_{\mathbf{k},\mathbf{k}'}^{CDW}$ of the itinerant 5f-quasiparticles have a purely electronic origin. We may have both unconventional SC with zero total pair momentum $\Delta_{\mathbf{k}}^0$ and at finite pair momentum $\Delta_{\mathbf{k}}^{\mathbf{Q}}$. The CDW gap function is denoted by $W_{\mathbf{k}}$ and like $\Delta_{\mathbf{k}}^0$ or $\Delta_{\mathbf{k}}^{\mathbf{Q}}$ belongs to an irreducible representation of the tetragonal D_{4h} group (this is also the approximate symmetry of UGe_2).

To treat both SC and CDW order parameters in a compact manner we introduce a Nambu-type representation using the spinors $\Psi_{\mathbf{k}}^{\dagger} = (c_{\mathbf{k}}^{\dagger}, c_{-\mathbf{k}}, c_{\mathbf{k}+\mathbf{Q}}^{\dagger}, c_{-\mathbf{k}-\mathbf{Q}})^{\dagger}$. Accordingly we use the tensor products $\hat{\rho} = (\hat{\sigma} \otimes \hat{I})$ and $\hat{\sigma} = (\hat{I} \otimes \hat{\sigma})$ for the Nambu representation of the Hamiltonian in Eq. (1). We assume that nesting in the fully FM polarized band is responsible for the CDW transition associated with the T^* line in UGe_2 . Pressure reduces T^* because it relaxes the nesting conditions. To model this effect we write the electron dispersion as a sum of particle-hole symmetric terms responsible for nesting and particle-hole asymmetric terms that represent the deviations from nesting: $\xi_{\mathbf{k}} = \gamma_{\mathbf{k}} + \delta_{\mathbf{k}}$ where $2\gamma_{\mathbf{k}} = \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{Q}}$ and $2\delta_{\mathbf{k}} = \xi_{\mathbf{k}} + \xi_{\mathbf{k}+\mathbf{Q}}$. When $\delta_{\mathbf{k}} = 0$ there is particle-hole symmetry or perfect nesting with wavevector \mathbf{Q} . Application of pressure adds a $\delta_{\mathbf{k}}$ term in the dispersion in addition to the $\gamma_{\mathbf{k}}$ term already present at zero pressure. We classify the SC and CDW order parameters with respect to their behavior under inversion (I) $\mathbf{k} \rightarrow -\mathbf{k}$, translation ($t_{\mathbf{Q}}$) $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{Q}$ and time reversal (T) in the charge sector. Instead of the latter we may also use complex conjugation (C) which satisfies the equivalence relations $C \equiv -T$ ($\Delta_{\mathbf{k}}^0$); $C \equiv IT$ ($\Delta_{\mathbf{k}}^{\mathbf{Q}}$) or $C \equiv t_{\mathbf{Q}}$ ($W_{\mathbf{k}}$). These discrete transformations may then be used to classify the possible groups of competing SC/CDW order parameters. Obviously C is redundant for the three order parameters considered, but we include it in the notation for clarity.

Because the spins are frozen, the $\mathbf{q} = \mathbf{0}$ SC pair states may only have odd parity with $\Delta_{-\mathbf{k}}^0 = -\Delta_{\mathbf{k}}^0$. Under

translation we have both signs $\Delta_{\mathbf{k}+\mathbf{Q}}^0 = \pm \Delta_{\mathbf{k}}^0$ and under C we get $(\Delta_{\mathbf{k}}^0)^* = -(\Delta_{\mathbf{k}}^0)^T = -\Delta_{\mathbf{k}}^0$. SC pair states with finite momentum may in principle have both parities: $\Delta_{-\mathbf{k}}^{\mathbf{Q}} = \pm \Delta_{\mathbf{k}}^{\mathbf{Q}}$ because the required antisymmetry may also come from the shift by a lattice vector \mathbf{R} with $\exp(i\mathbf{Q}\mathbf{R}) = -1$. On the other hand the $t_{\mathbf{Q}}$ translation requires that always $\Delta_{\mathbf{k}+\mathbf{Q}}^{\mathbf{Q}} = -\Delta_{\mathbf{k}}^{\mathbf{Q}}$ and under C we have $(\Delta_{\mathbf{k}}^{\mathbf{Q}})^* = (\Delta_{-\mathbf{k}}^{\mathbf{Q}})^T = -\Delta_{-\mathbf{k}}^{\mathbf{Q}}$. These transformation properties allow *four possible SC order parameters, two at zone center and two at zone boundary or staggered SC*: $\Delta_{\mathbf{k}}^{0I--}$, $\Delta_{\mathbf{k}}^{0I+-}$, $\Delta_{\mathbf{k}}^{\mathbf{Q}R--}$, $\Delta_{\mathbf{k}}^{\mathbf{Q}I+-}$. Here the first index $\mathbf{0}$ or \mathbf{Q} indicates the *total momentum of the pair*, the second index R or I indicates whether the order parameter is real or imaginary, the third index \pm indicates parity under inversion I and the last index denotes gap symmetry under $t_{\mathbf{Q}}$. As mentioned the index I(R) is redundant.

For the CDW order parameter both odd and even states under I and $t_{\mathbf{Q}}$ are allowed so that $W_{-\mathbf{k}} = \pm W_{\mathbf{k}}$ and $W_{\mathbf{k}+\mathbf{Q}} = \pm W_{\mathbf{k}}$ may hold. Since $C \equiv t_{\mathbf{Q}}$ for this order parameter the redundant index R or I is associated with the $t_{\mathbf{Q}}$ -index \pm respectively. As a result we have here again four different possible (CDW) order parameters: $W_{\mathbf{k}}^{R++}$, $W_{\mathbf{k}}^{I+-}$, $W_{\mathbf{k}}^{R-+}$, $W_{\mathbf{k}}^{I--}$, where the indices have the same meaning as the last three indices in the SC order parameters. According to the above symmetry classification there are *sixteen* possible pairs of such competing SC/CDW states and only *eight of them concern staggered SC* on which we are interested here. Within our formalism we can calculate Green's functions and self-consistent gap equations for each of these eight cases. As an example relevant for UGe_2 we report here for the case of the competition of $W_{\mathbf{k}}^{I+-}$ with $\Delta_{\mathbf{k}}^{\mathbf{Q}R--}$ where the Hamiltonian in spinor representation with Pauli matrices $\hat{\sigma}_i$ and $\hat{\rho}_i$ is $H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \hat{\Xi}_{\mathbf{k}} \Psi_{\mathbf{k}}$ where $\hat{\Xi}_{\mathbf{k}} = \gamma_{\mathbf{k}} \hat{\rho}_3 \hat{\sigma}_3 + \delta_{\mathbf{k}} \hat{\sigma}_3 + \Delta_{\mathbf{k}}^{\mathbf{Q}R--} \hat{\rho}_2 \hat{\sigma}_2 - W_{\mathbf{k}}^{I+-} \hat{\rho}_2$. We note that if instead of having the competition of $W_{\mathbf{k}}^{I+-} \hat{\rho}_2$ with $\Delta_{\mathbf{k}}^{\mathbf{Q}R--} \hat{\rho}_2 \hat{\sigma}_2$ as above, we had any of the other pairs of competing order parameters, we would just have to replace the corresponding SC and CDW terms in the above Hamiltonian. The Green's functions that result would be modified accordingly. For the $W_{\mathbf{k}}^{I+-} \hat{\rho}_2$ and $\Delta_{\mathbf{k}}^{\mathbf{Q}R--} \hat{\rho}_2 \hat{\sigma}_2$ order parameters, the most obvious realization in D_{4h} symmetry is a d-wave CDW and p-wave (finite momentum) SC order parameter given by $\Delta_{\mathbf{k}}^{\mathbf{Q}} = \Delta_{\mathbf{0}}^{\mathbf{Q}} (\sin k_x + \sin k_y)$ (i.e. $E_u(1,1)$) and $W_{\mathbf{k}} = W_0 (\cos k_x - \cos k_y)$ (i.e. B_{1g}). From the Hamiltonians we obtain Green's functions and then self-consistent gap equations for both order parameters which after analytic summation over the Matsubara frequencies take the form of the following system of coupled equations that are reported for the first time here:

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} \frac{V_{\mathbf{k},\mathbf{k}'}^{SC} \Delta_{\mathbf{k}'}}{4\sqrt{\delta_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2}} \left[\tanh \frac{E_+(\mathbf{k}')}{2T} - \tanh \frac{E_-(\mathbf{k}')}{2T} \right] \quad (2)$$

$$W_{\mathbf{k}} = \sum_{\mathbf{k}'} \frac{V_{\mathbf{k},\mathbf{k}'}^{CDW} W_{\mathbf{k}'}}{4\sqrt{\gamma_{\mathbf{k}'}^2 + W_{\mathbf{k}'}^2}} \left[\tanh \frac{E_+(\mathbf{k}')}{2T} + \tanh \frac{E_-(\mathbf{k}')}{2T} \right] \quad (3)$$

$$E_{\pm}(\mathbf{k}) = \sqrt{\gamma_{\mathbf{k}}^2 + W_{\mathbf{k}}^2} \pm \sqrt{\delta_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} \quad (4)$$

Here the effective potentials $V_{k,k'}^{SC}$, $V_{k,k'}^{CDW}$ are separable for the assumed E_u and B_{1g} channels. If solutions of these coupled SC/CDW gap equations exist they are unique. For uniform order parameters assumed here they also have lower free energy as compared to the normal state [22,23]. Eqs. (2,3) account for the following *four* pairs of competing CDW and zone boundary states: Δ^{RQ-} with W^{R++} , Δ^{RQ-} with W^{I+-} , Δ^{IQ-} with W^{R++} and Δ^{IQ-} with W^{I+-} . There is a second system of coupled gap equations that describes the competition of the *remaining four* pairs of SC and CDW gaps: Δ^{RQ-} with W^{R-+} , Δ^{RQ-} with W^{I--} , Δ^{IQ-} with W^{R-+} and Δ^{IQ-} with W^{I--} :

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{SC} \Delta_{\mathbf{k}'} \left\{ \frac{B(\mathbf{k}) + \gamma_{\mathbf{k}'}^2}{4E_+(\mathbf{k}')B(\mathbf{k})} \tanh \left[\frac{E_+(\mathbf{k}')}{2T} \right] + \frac{B(\mathbf{k}) - \gamma_{\mathbf{k}'}^2}{4E_-(\mathbf{k}')B(\mathbf{k})} \tanh \left[\frac{E_-(\mathbf{k}')}{2T} \right] \right\} \quad (5)$$

$$W_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{CDW} W_{\mathbf{k}'} \left\{ \frac{B(\mathbf{k}) + \delta_{\mathbf{k}'}^2}{4E_+(\mathbf{k}')B(\mathbf{k})} \tanh \left[\frac{E_+(\mathbf{k}')}{2T} \right] + \frac{B(\mathbf{k}) - \delta_{\mathbf{k}'}^2}{4E_-(\mathbf{k}')B(\mathbf{k})} \tanh \left[\frac{E_-(\mathbf{k}')}{2T} \right] \right\} \quad (6)$$

where

$$E_{\pm}(\mathbf{k}) = \sqrt{\frac{\Delta_{\mathbf{k}}^2 W_{\mathbf{k}}^2}{\gamma_{\mathbf{k}}^2 + W_{\mathbf{k}}^2} + \left[\sqrt{\gamma_{\mathbf{k}}^2 + W_{\mathbf{k}}^2} \pm \sqrt{\frac{B(\mathbf{k})}{\gamma_{\mathbf{k}}^2 + W_{\mathbf{k}}^2}} \right]^2} \quad (7)$$

$$B(\mathbf{k}) = \sqrt{\delta_{\mathbf{k}}^2 (\gamma_{\mathbf{k}}^2 + W_{\mathbf{k}}^2) + \gamma_{\mathbf{k}}^2 \Delta_{\mathbf{k}}^2} \quad (8)$$

We have solved selfconsistently the systems of Eqs. (2,3) and (5, 6) for a 2D tight-binding model on a square lattice. In that case, the particle-hole symmetric term corresponds to nearest neighbor hopping $\gamma_{\mathbf{k}} = t_1(\cos k_x + \cos k_y)$ while particle-hole asymmetry is introduced by the next-nearest neighbor hopping terms $\delta_{\mathbf{k}} = t_2 \cos k_x \cos k_y$. We have performed a large number of self consistent calculations varying the pairing potentials in the two channels producing eight maps (two of them reported in figure 1) of *all possible transitions induced by particle-hole asymmetry (i.e. by pressure)* in the low- T region for all the pairs of competing CDW and staggered SC order parameters that are possible. To take into consideration the fact that the different CDW and SC gap symmetries involved may correspond to different momentum structures for the order parameters, we have considered the separable potentials approximation that allows to search for solutions of a specific momentum structure. Therefore, the axes in Fig.1 are the amplitudes V^{CDW} and V^{SC} of the pairing interactions and it is understood that a corresponding form factor has been considered. We have investigated the coexistence of order parameters in the whole (V^{CDW}, V^{SC}) plane from the moderate coupling to the strong coupling regime since we have no microscopic derivation for the effective pairing

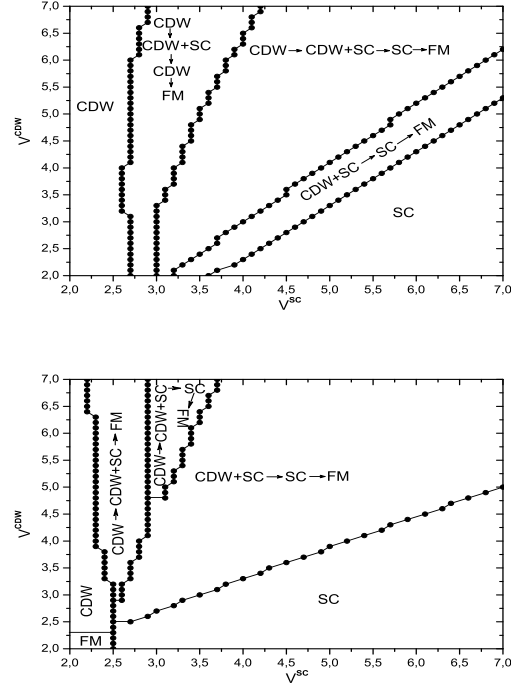


Fig. 1: Maps of the dependence of phase sequences on the effective interactions V^{CDW} and V^{SC} for low temperature. Arrows indicate the cascade of phases obtained when t_2/t_1 grows starting from zero. The black dots separate regions of different phase *sequences* under growing t_2/t_1 . All phases coexist with ferromagnetism (FM). The phases indicated as FM, are phases in which there is not any finite SC or CDW order parameter and so only FM is present. Figure a) corresponds to the competition of Δ^{RQ--} with W^{I--} . Figure b) corresponds to the competition of Δ^{RQ--} with W^{R-+} . The potentials are in units of t_1 .

strengths. Arrows in Fig. 1 indicate the cascade of phases observed when the ratio t_2/t_1 grows starting from zero. Since we consider a spin polarized background, all states reported also coexist with FM, and the transitions to the FM state reported at high values of t_2/t_1 has the meaning of a transition to a state that is only ferromagnetic with no CDW or SC order parameter present. We note in figure 1a that in a large portion of the V^{SC}, V^{CDW} parameter space there is at low temperature a transition from a CDW state to a state in which CDW and SC coexist. The same transition is also present over a portion of the parameter space in the case of figure 1b. We note that the coexistence of zone-center SC with CDW has been reported in previous theoretical studies [22,27,28].

We now look more closely to the situations in which CDW and staggered SC may coexist. We report in figure 2a the behavior of the CDW+SC state with t_2/t_1 in a characteristic example that corresponds to $V^{CDW} = 4$ and $V^{SC} = 2.5$ in the competition of Δ^{RQ--} with W^{R-+} at low- T the mapping of which is reported in figure 1b. We observe the cascade of transitions from CDW to CDW+SC

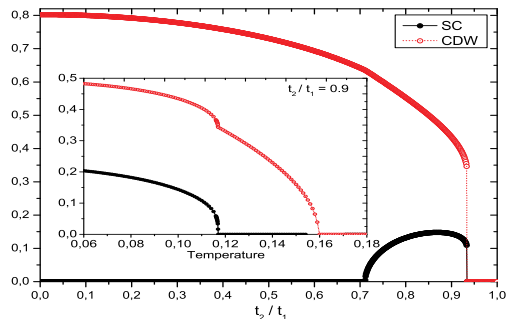


Fig. 2: (Color online): A characteristic example in which deviations from nesting induced by t_2/t_1 lead to coexistence of the W^{R-+} CDW (open circles in red) with the Δ^{RQ--} staggered SC order parameter (filled circles in black) corresponding to $V^{CDW} = 4$ and $V^{SC} = 2.5$. We observe the cascade of transitions from CDW to CDW+SC and then to FM as was already reported in figure 1b in this region of V^{CDW} and V^{SC} values. In the inset is shown the temperature dependence of both order parameters when $t_2/t_1 = 0.9$ in which case the CDW and SC orders coexist at low temperatures. All quantities are in units of t_1 .

at $t_2/t_1 \approx 0.72$ and finally to the FM state for $t_2/t_1 > 0.93$ in agreement with the cascade reported in figure 1b for these couplings. It is remarkable in figure 2a that the transition from CDW to CDW+SC is smooth as a function of t_2/t_1 in the low-T regime whereas the transition from the CDW+SC state to the FM state (i.e. the state with no SC or CDW) is first order in t_2/t_1 . In figure 2b we show the corresponding transitions with temperature when we take $t_2/t_1 = 0.9$. In this case, according to figure 2a, we have indeed in low-T coexistence of CDW and SC. We observe the counter-intuitive behavior that when SC appears as we lower the temperature, the CDW gap grows instead of being reduced.

A particularly interesting cascade of transitions in relation to the observations in UGe_2 , is the one from CDW to CDW+SC to SC and finally to FM. This cascade is observed over a large portion of the parameter space of pairing potentials when the Δ^{RQ--} and W^{I--} compete (cf. fig. 1a) and over a smaller portion in the case of competition of Δ^{RQ--} with W^{R-+} (fig. 1b). A cascade of transitions in the low temperature regime that exhibits amazing similarities with that observed in UGe_2 as a function of pressure is shown in Fig.3. It corresponds to the competition of W^{R-+} CDW with the staggered SC order of the form Δ^{RQ--} when $V^{SC} = 3.5$ and $V^{CDW} = 12.5$. The maximal critical temperature of SC coincides with the crossing of the CDW critical line. Moreover, the SC dome is divided into a part in which SC and CDW coexist and a part in which only SC is present (with FM of course). Quite remarkably the SC critical temperature is reduced almost linearly at the higher values of t_2/t_1 . The above results are in surprising qualitative agreement with

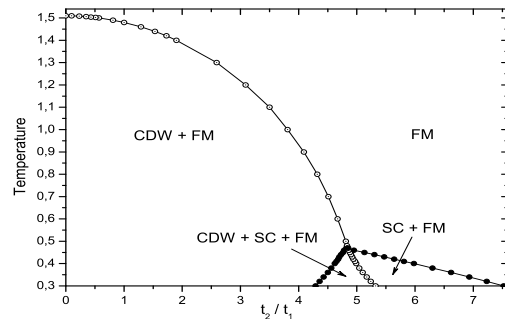


Fig. 3: Evolution with temperature of a cascade of t_2/t_1 induced transitions from CDW to CDW+SC to SC and then to only FM obtained when $V^{CDW} = 12.5$ and $V^{SC} = 3.5$. The SC and CDW order parameters considered are Δ^{RQ--} and W^{R-+} . This phase diagram shows striking similarities with features of the pressure phase diagram of UGe_2 if one suppose that the T^* phase corresponds to a W^{R-+} CDW ordering and of course SC to Δ^{RQ--} .

findings in UGe_2 [18]. In particular, recent NQR results indicate that the T^* phase coexists indeed with SC over a portion of the SC dome [19] and our results are the first to provide a theoretical picture for it.

Staggered SC states are relevant for magnetic SC [20,24, 25] because they are similar to the Fulde-Ferrel states [26] except that the modulation of the superfluid density coincides with the characteristic wavevector of the CDW. It appears, therefore, plausible to consider these states in the analysis of SC in UGe_2 which is observed only in the FM regime because for a staggered SC the FM background is necessary in the same way as the magnetic field is necessary in order to obtain the usual Fulde-Ferrel phase. Since pressure eliminates the FM state it naturally eliminates simultaneously the staggered SC state as well. Note finally that we obtain staggered SC states only over a *limited dome* near the collapse of the CDW phase as in figures 2 and 3 *within a mean field approach without any fluctuations involved*.

In conclusion, we have demonstrated the possibility to have *coexistence of staggered SC with CDW* and cascades of transitions induced by particle-hole asymmetry that reproduce the pressure phase diagram observed in UGe_2 identifying the T^* phase as a CDW phase. Such exotic states may be relevant for other magnetic SC as well.

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